

Summary of Updates & Changes in BatPaC 5.0

This document provides a list of the modifications and improvements made from BatPaC 4.0 to BatPaC 5.0. Full details will be published in the 4th edition of the BatPaC manual to be released in 2022.

Improvements to Calculations and Default Values

1. *Redesign of cell, module, and pack* – modifications were made to the assumed cell, module, and pack design to better align with observed best-practices in industry. This includes changes to the cell terminal, cell tabs, cell interconnections within the module, module tabs, module management system, assembly of modules in pack, and coolant management within the pack.
2. *Redesign of the manufacturing plant* – the cost of a manufacturing plant was revised using new data. This includes changes to the capital equipment costs, labor, plant size, plant utilities, and scaling factors. The calculation was also modified to properly account for changes in manufacturing costs due to changes in the estimated plant operational days per year.
3. *Improvements to fast charging* – a combined thermal-electrochemical model was used to develop correlations which restrict cell design based on fast-charging requirements. Details of the study were recently published in Energy and Environmental Sciences (DOI: [10.1039/D1EE02286E](https://doi.org/10.1039/D1EE02286E)). These correlations are used in the pack design when “Fast Charging” is selected for electric vehicles on the “Dashboard” tab.
4. *Default cells for power and energy* – each default chemistry now includes two default options for cell design based on either power or energy applications. The power and energy designs differ in electrode porosity, active material particle size, carbon additive weight percent, and current collector thickness. These values impact the area specific impedance used in the battery design.
5. *BMS model updates* – the battery management system (BMS) model was updated so the design and corresponding properties (volume, weight, and cost) of the BMS depend on the current and voltage of the battery pack. Additionally, it is now assumed that the BMS is fabricated in-house with the pack. Therefore, profits and overhead associated with purchasing the BMS from a third party have been removed.
6. *Self-consistent default properties* – the default active material capacities and cell open circuit voltages were updated to guarantee self-consistency between the capacities of the materials, the voltage of the cell, the desired negative-to-positive capacity ratio after formation, and the anticipated formation losses of the materials. The calculations were accomplished using a new tool made available to the users in BatPaC 5.0 (see #13).

Additions to User Functionality

7. *ASI as a function of temperature* – the area specific resistance (ASI) of the cells can be adjusted based on the operating temperature of the pack, which is set by the user in the

“Dashboard” tab. This is accomplished using an Arrhenius equation with constants obtained from experimental tests run at the Cell Analysis, Modeling, and Prototyping (CAMP) facility at Argonne.

8. *Pack designs for exceptional power requirements* – the user can now select the pulse length (seconds) and state of charge (SOC, %) that determine the power requirements of the pack. This makes it possible to design battery packs using the default chemistries for unique power requirements not included in the default vehicle types. Previously, the length and SOC were built into the selection of the vehicle type. For instance, the power of a 100% electric vehicle was designed using the ASI and open circuit voltage (OCV) from a 30-second pulse at 20% SOC. The default ASI and OCV values for the vehicle types remain in BatPaC 5.0. However, the user can also modify the ASI and OCV by changing the desired pulse length and state of charge. This is accomplished using a correlation developed from simulated results generated for a wide range of chemistries, electrode loadings, pulse lengths, SOC, and discharge powers.
9. *Plant utilization* – the cost of manufacturing the battery packs can be modified depending on the utilization of the plant. Two options for under-utilization are provided in the “Dashboard” tab: *i)* the plant is built for full capacity but operated at part-capacity and *ii)* the space is provided for full-scale production, but equipment is provided only for the initial part-production level.
10. *Manufacturing method* – the manufacturing cost calculation can be modified to account for three pack-manufacturing scenarios: *i)* all manufacturing from cells to modules to packs is done in-house, *ii)* the cells are purchased from a 3rd party vendor and used to manufacture the modules and packs, and *iii)* the modules are purchased from a 3rd party vendor and used to manufacture the packs. Each scenario impacts the investment and materials costs incurred by the pack manufacturer. Materials purchased from 3rd party vendors include price mark-ups for profit and warranty.
11. *Pack cost options* – the user can now select whether the displayed pack costs include profits and warranty (referred to as “Cost to Consumer”) or not (referred to as “Cost to Build”)
12. *Additives in cell* – the “Chem” tab was modified so the user can include additives in the negative electrode, positive electrode, and electrolyte formulations. The cost and weight of the additives are included in the final pack design metrics.
13. *Tool for generating new chemistry couples* – a new tool was created for generating the properties of new chemistry couples that can be modeled by BatPaC. The tool is in the “Tool-Generate Chem Couple” tab. The user can select electrode chemistries for the positive and negative electrodes from a database, the desired negative-to-positive (N2P) capacity ratio after formation, the open circuit voltage (OCV) at 100% state of charge (SOC) and any losses during formation. The tool uses a database of voltage versus capacity values for each chemistry, along with the user inputs, to calculate the reversible capacities (mAh/g) of the positive and negative materials and the OCV versus SOC. The tool makes sure the capacity and OCV values are self-consistent with the desired N2P ratio and voltage

window set by the user. The capacity and OCV can be used to build new chemistry couples in the “Chem” tab. See below for a guide on how to use the new tool.

14. *Adding new vehicle types* – BatPaC 5.0 includes the ability to add new vehicle types through the “Vehicle Considerations” tab. This tab contains a table for each vehicle type and lists the design properties and BMU/thermal considerations that are unique for each vehicle, which are called upon in the model. Additional vehicles (*e.g.*, trucks, SUVs, aerial vehicles, and forklifts) can be modeled by adding a new column to the table and inputting the correct properties and considerations in the designated rows. Additional vehicles are automatically updated to the vehicle pull-down menu on the “Dashboard” tab.

Enhancements to User Interface and Results

15. *Updates to Dashboard* – the “Dashboard” tab has been revised to include the features described above. This includes override options for peak power duration and SOC at rated power, inputs for operating temperature, and a region to modify plant utilization and cell yield. Also, the ability to specify the storage size of the vehicle was simplified to either capacity (Ah) or energy (kWh). Previous versions also included the ability to specify storage by combining the Wh/mile of the vehicle and the desired range (miles). This option was removed to prevent confusion by reducing the number of parameters and options available to the user. In addition, air cooling was eliminated from the default cooling options on the Dashboard.
16. *Updates to “Chem” tab* – additional detail was included on the electrochemical properties, including the area specific impedances and open circuit voltages from 0-100% state of charge in increments of 10%. This information is used for modeling exceptional power requirements. Additional calculations were also provided for the interfacial resistance of the default couples to provide clarity for the user and to serve as a reference point for the creation of new couples.
17. *Scrap material and recycling* – the “Recycle” tab was expanded to include the materials that could be recovered as scrap during the manufacturing process (*e.g.*, waste from mixing, coating, slitting, etc.). The tab was further expanded to include the option to track the masses of up to four elements that exist in the cells and packs.

Comparison Between BatPaC 4.0 and 5.0 Results

This section demonstrates how changes from BatPaC 4.0 to 5.0 affect the predicted cost and performance metrics of electric vehicle battery packs. The demonstration is designed to highlight the nuances associated with comparing 4.0 to 5.0. Significant changes were made between the versions. Therefore, reasons behind the changes in results from 4.0 to 5.0 are not always straightforward. Insight will be provided from the new manual that is forthcoming.

A comparison was conducted between BatPaC 4.0 and 5.0 for battery packs intended for high-power hybrid-electric vehicles (HEV-HPs) and all electric vehicles (EVs). All calculations were done using the default costs and properties from each BatPaC version for a pack with NMC811-

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graphite cells. The total pack costs include profits and warranty that would be passed on to the consumer.

The results of the comparison are shown in Figure 1. Figure 1a compares the cost (\$/kWh), specific energy (Wh/kg), and energy density (Wh/L) for packs and cells in a nominal HEV-HP pack. Results are shown for a 125 kW/5 kWh pack manufactured in a plant with a 2.5-GWh/year (500,000-pack/year) capacity. The BatPaC 5.0 results were calculated using the “power” couple for NMC811-G since this is a high-power application with an energy-to-power ratio equal to 25 (see #4 above for a brief discussion). The total pack cost decreases from \$334 to \$270/kWh from BatPaC 4.0 to 5.0. This is mainly due to modifications in the BMS and a reduction in the cell cost from \$139 to \$104/kWh. The cell cost decreases due to improvements in the area specific impedance (ASI) of the “power” couple and a reduction in the default cost of the separator from \$1.1 to \$0.9/m².

Both the weight and size of the HEV-HP pack increase from BatPaC 4.0 to 5.0, as exemplified by the decreases in Wh/kg and Wh/L, respectively. On the cell level, the mass increase is mainly due to increased current collector thicknesses designed to reduce ASI in the “power” couple. The increase in cell size is caused by tab modifications, which ease the connection between cells but occupy more volume in the module. These increases in weight and size of the cell propagate to the pack. The pack also adds size and weight with the addition of a cooling panel and a revised support system to improve thermal control and structural stability, respectively.

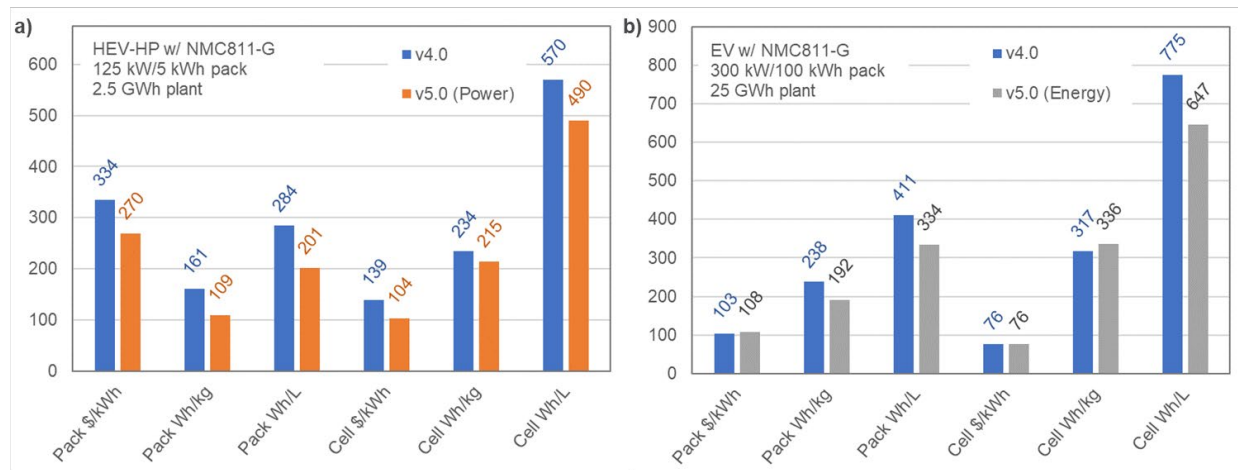


Figure 1. Comparison of default results from BatPaC 4.0 and BatPaC 5.0 for a) a nominal high power pack in a hybrid-electric vehicle (HEV-HP) and b) a nominal pack in an all electric vehicle (EV). Cells were NMC811-graphite. All other relevant properties can be found on the plot.

Figure 1b compares the pack designs for a 300 kW/100 kWh EV built in a 25-GWh/year (250,000-pack/year) plant. The increases in the size of the pack and cell (decreases in Wh/L) and increase in the weight of the pack (decrease in Wh/kg) are caused by the cell-tab and pack re-designs mentioned in the preceding paragraph. The decrease in cell weight (increase in Wh/kg) is due to a reduction in the mass of the tab and the use of the “energy” couple, which has thinner current collectors than the “power” couple. A similar reduction in tab mass was observed for the HEV-HP, but it was not high enough to offset other gains.

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The cell cost remained the same (~\$76/kWh) for the EV from BatPaC 4.0 to 5.0. This is in contradiction to the HEV-HP cells, which demonstrated a decrease in cost primarily due to decreases in the separator cost. The HEV-HP cells have thinner electrodes (with more separator area) to reach high power. This design makes items priced on a $\$/\text{m}^2$ basis (like the separator) more important in HEV-HP cells. For the EV cells, the decreases in separator cost were balanced out by increases in the NMC811 cost from \$22 to \$26/kg, keeping the total cell cost the same. Finally, increases in the cost of the pack from \$103 to \$108/kWh are primarily due to the propagation of the increase in cell cost and an increase in the manufacturing cost due to increased capital expenditures in the revisited plant design. Note that the BMS, which is partly responsible for the decrease in HEV-HP pack cost, is not a strong driver to reduce the EV pack cost because it only accounts for ~3% of the cost. For the HEV-HP, the BMS is ~30% of the total cost due to similar per-pack prices for contactors and disconnects regardless of the kW and kWh rating.

Guide for using “Tool-Generate Chem Couple”

The tab “Tool-Generate Chem Couple” provides a tool for generating the properties – *i.e.*, reversible gravimetric capacities of the active materials (mAh/g) and open circuit voltage (OCV) versus state of charge (SOC) – of new chemistry couples that can be modeled with BatPaC. The tool guarantees the capacity and OCV values are self-consistent with the desired negative-to-positive capacity ratio and voltage window set by the user.

First, macros must be enabled on the workbook to use the tool. To enable macros in Excel, select “Developer” in the ribbon (Figure 2). Then choose “Macro Security” and make sure “Enable all macros” is selected in the pop-up window that appears. Click “OK” once this is confirmed. Next, follow the four steps outlined below to create a new couple and output the results to the “Chem” tab.

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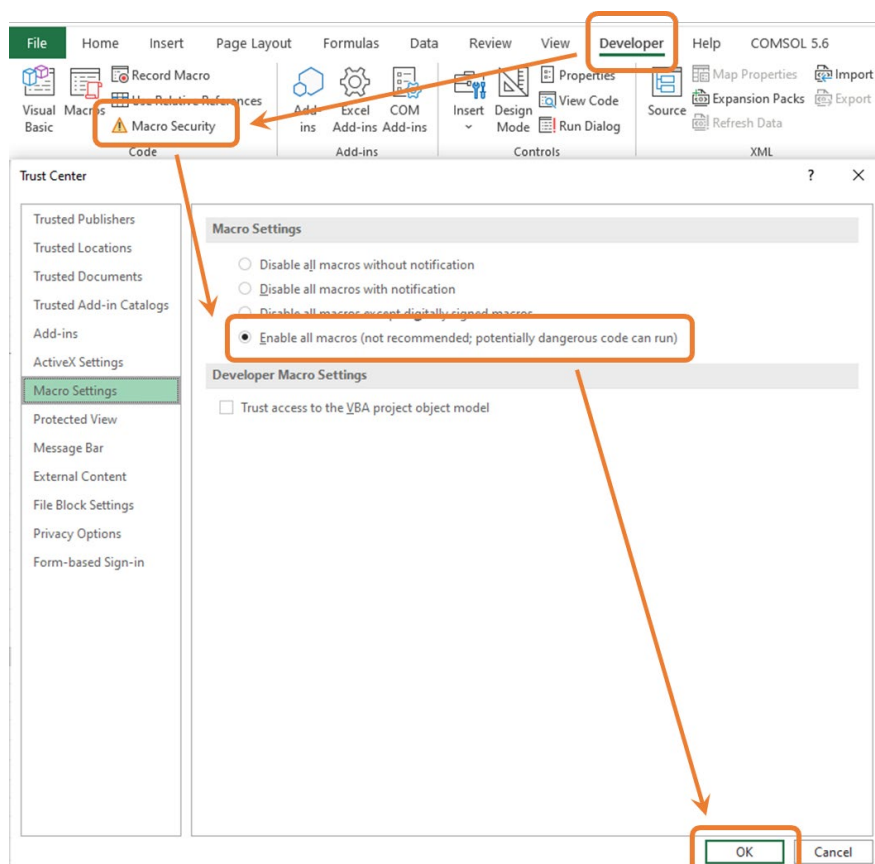


Figure 2. Image showing how to enable macros in Microsoft Excel.

Step 1: Choose couple and formation information

The active materials in the new couple are chosen either by taking the values from the currently selected chemistry couple, which was selected on “Dashboard” (Figure 3a) or by creating a new couple from a database of active materials provided by BatPaC (Figure 3b). Use the drop-down menu next to the “Select Method” cell to choose one of the two options. If the first option is chosen, the positive and negative electrode chemistries are automatically taken from the currently selected values on Dashboard. If the second option is chosen, two drop-down boxes appear, which must be used to select the chemistries from a database of values. Results are only guaranteed when graphite (G) or lithium titanate (LTO) are used as the negative electrode. If any other chemistry is selected as the negative electrode or either of the two are chosen as the positive, a warning message shows up in the “Check for compatibility” rows.

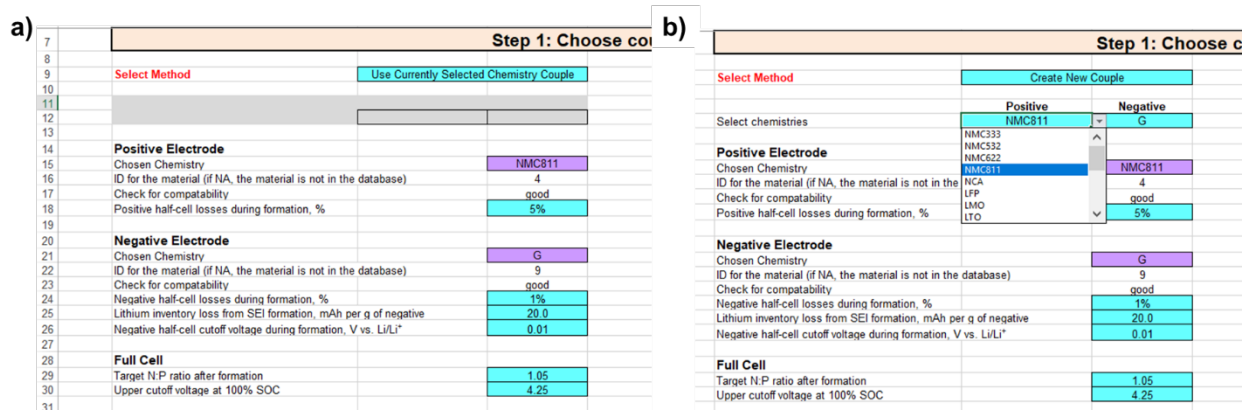


Figure 3. Screenshots showing two ways to choose the new chemistry couple when using the tool: a) by using the currently selected chemistry couple from “Dashboard” and b) by creating a new couple from the database.

Next, input information on the three expected capacity losses during formation. The first is the positive half-cell losses during formation, which reflects the loss in active sites of the positive material during formation and has units of percent of first cycle capacity. The second is the negative half-cell losses during formation, which reflects the loss in active sites of the negative material during formation and has units of percent of first cycle capacity. Both values should be provided without regards to lithium inventory loss. They should reflect the losses observed during formation of half-cells with excess Li-metal, where the voltage windows for either electrode are identical to the voltage windows observed during operation of the full cell when measured with respect to a Li/Li⁺ reference electrode. The third loss is the lithium inventory loss from SEI formation. It has units of mAh of lithium lost per gram of negative active material. The description assumes all lithium inventory loss occurs at the negative electrode SEI, which was done for simplicity. Other forms of lithium inventory loss (*e.g.*, cathode-electrolyte interphase, CEI) can be incorporated by increasing the value of this term.

In addition to formation losses, specify the desired negative half-cell cutoff voltage during formation. This sets the lowest voltage seen by the negative electrode when the full cell is at 0% SOC. The upper cutoff voltage of the full cell at 100% SOC must also be provided to set the voltage window. Finally, specify the target negative-to-positive capacity ratio in the full cell after formation.

Step 2: Run Calculation

Click the button to initiate the macro, which will run the calculation (Figure 4).

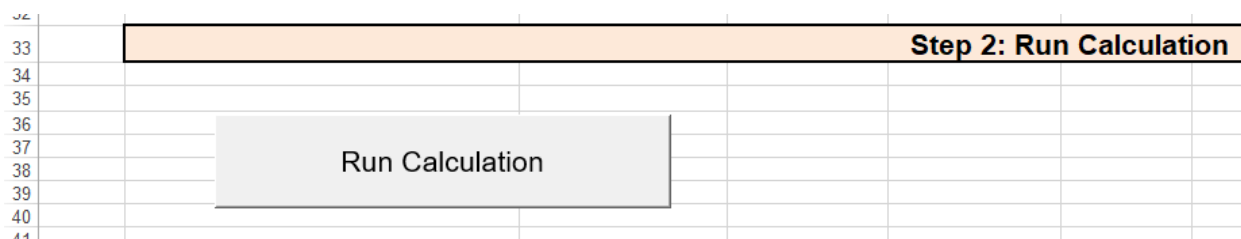


Figure 4. Screenshot showing the button to run the calculation

Step 3: Verify/modify output data

The results of the calculation (*i.e.*, gravimetric capacities, N:P ratio, and OCV vs. SOC) will appear in the table as shown in Figure 5. This section also includes a graph of the OCV vs. SOC for the full cell. Verify the results and repeat steps 1 and 2 until satisfied. If necessary, override the calculated voltage using column E. However, this is only advised for minor changes (*e.g.*, adjusting the calculated OCV at 0% SOC from 3.01 to 3.00 to yield a more typical lower cutoff voltage).

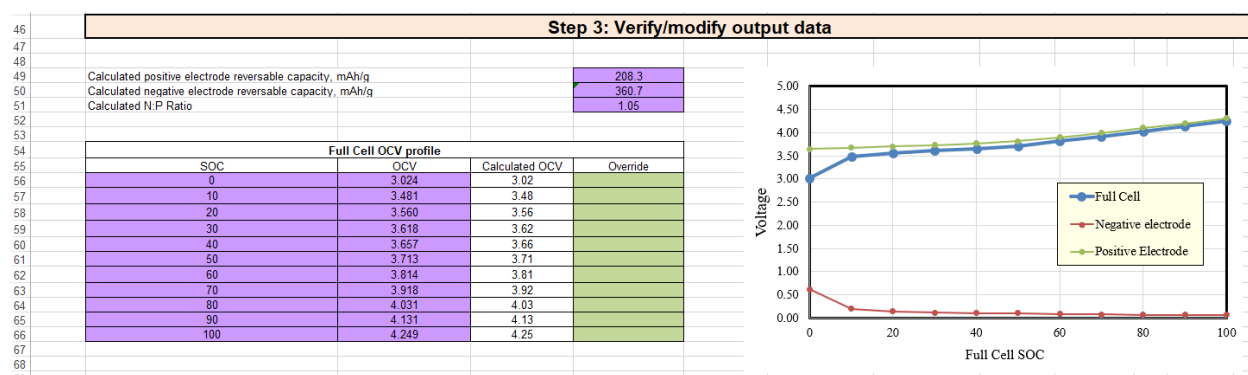


Figure 5. Screenshot showing the results of the calculation.

Step 4: Export to Chem Tab

Two options are provided for transferring the results to the “Chem” tab to be used by BatPaC for the battery design calculation (Figure 6). For the first option, click the button labeled “Add Values to Current.” This will add the new values to the override column in the “Chem” tab. All other properties come from the existing, default electrode couple selected in “Dashboard”, unless overridden previously.

The second option is to create a new default chemistry couple that will be added to the list of selectable chemistry couples in the electrode couple drop-down menu on “Dashboard.” First, use the drop-down list under “Select a Chemistry Couple to Use to Serve as Template” to select a pre-existing default couple to serve as template. Next, provide a name for the new couple under “Create Name for New Electrode Couple.” An error will appear if the name already exists. After that, click the button “Create New Electrode Chemistry Couple” to add the new couple to the default list. The

couple will be created by combining the calculated results above with all other properties from the template couple (e.g., ASI, densities, porosities, etc.). Finally, to use the new couple in the BatPaC calculations, return to “Dashboard” and select the new couple in the electrode couple pull-down menu.

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Step 4: Export to Chem Tab
Choose option 1 or option 2

Option 1: Update values for the currently selected chem couple
Values will be placed in the override column in the Chem tab (ChemE)

Parameter	Current Default Values	Updated Values	Current Overrides
Positive electrode reversible capacity, mAh/g	213.60	207.97	0.000
Negative electrode reversible capacity, mAh/g	360	360.74	0.000
N:P ratio	1.10	1.10	0.000
OCV at 0% SOC, V	3.000	3.026	0.000
OCV at 10% SOC, V	3.479	3.479	0.000
OCV at 20% SOC, V	3.556	3.556	0.000
OCV at 30% SOC, V	3.617	3.617	0.000
OCV at 40% SOC, V	3.658	3.658	0.000
OCV at 50% SOC, V	3.713	3.713	0.000
OCV at 60% SOC, V	3.809	3.809	0.000
OCV at 70% SOC, V	3.916	3.916	0.000
OCV at 80% SOC, V	4.032	4.032	0.000
OCV at 90% SOC, V	4.131	4.131	0.000
OCV at 100% SOC, V	4.250	4.250	0.000

Should be the same after running macro

Option 2: Create new default chem couple
OCV, capacity, and N2P values will be replaced; all other values will be copied from the template chemistry couple

Select a Chemistry Couple to Use to Serve as Template
Chemistry Couple as Template: NMC333-G (Power)

Create Name for New Electrode Couple
New Couple Name: NMC532-G-Add_test
*** Check Name capatability: no problems

Create New Electrode Chemistry Couple

Add Values to Current

Figure 6. Screenshot showing the two options for exporting the results to the Chem tab.

Explanation of Calculation

The calculation is solved using two, nested, iterative loops to guarantee self-consistency between all parameters. Two flow charts are provided below to describe the calculation. The full calculation is contained at the end of the spreadsheet.

The outer loop is shown by the flow chart in Figure 7. Here, the positive, first-charge, cutoff voltage is iteratively updated until the full cell voltage at 100% state of charge (SOC) converges to the target value. The positive, first-charge, cutoff voltage is used to determine the gravimetric capacity of the positive material. It is used in combination with the user-specified formation losses and the negative voltage at 0% SOC (see input arrows in Figure 7) to solve the inner, iterative loop shown by Flow Chart 2 in Figure 8.

The inner loop (Figure 8) iteratively updates the negative-to-positive (N:P) mass ratio until the N:P capacity ratio converges to the target value. At first, the user-specified, positive site losses; the positive, first-charge cutoff voltage specified by the outer loop; and the positive mAh_{theory}/g vs.

OCV (*i.e.*, no losses) are used to determine the positive reversible, half-cell capacity. Next, the total number of positive sites lost (in mAh) is calculated using this value and the N:P mass ratio. This is compared to the Li inventory losses (in mAh) calculated from the N:P mass ratio and the user-specified mAh lost per gram of negative. The relative size of the positive losses and Li inventory losses determines the course of action for calculating the real capacity of each material in the full cell. If the positive site losses are larger, the negative capacity is adjusted to account for the fact some lithium will reside in the negative upon discharge because it has no “home” in the positive. If the Li inventory losses are greater, the positive capacity is adjusted to account for a lack of Li to fill all its vacant sites upon discharge. Simultaneously, the reversible, half-cell capacity of the negative material is calculated using the user-specified, negative site losses; the user-specified negative voltage at 0% SOC; and the BatPaC-provided mAh_{theory}/g vs. OCV. Both reversible capacities are combined with the adjustments to determine the mAh/g. The calculated mAh/g are then combined with the N:P mass ratio to determine the N:P capacity ration. Finally, this value is compared with the target and the N:P mass ratio is updated.

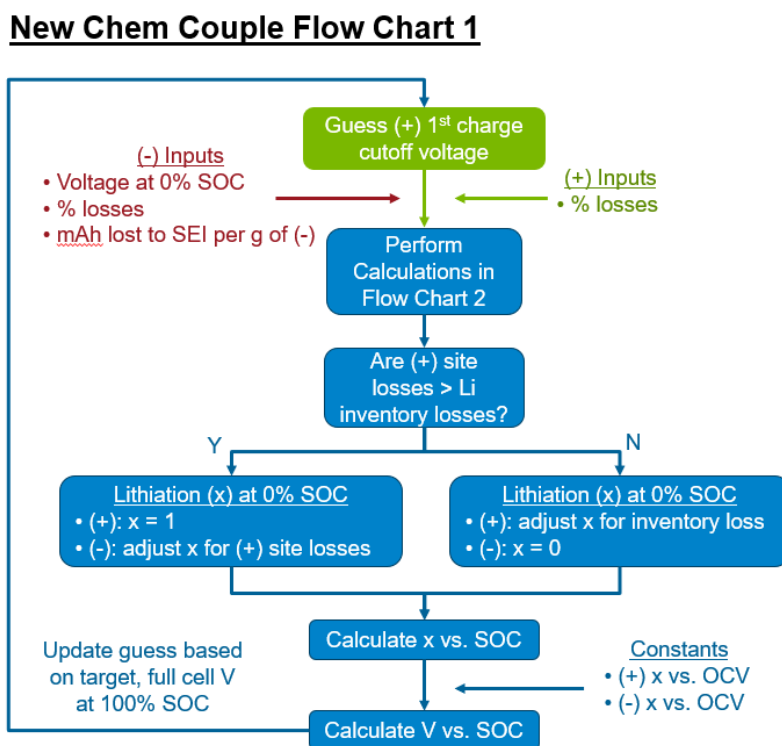


Figure 7. Flow chart describing the outer iterative loop in the calculation. The positive first-charge cutoff voltage is updated iteratively in the calculation until the full cell voltage at 100% state of charge converges to the target value. OCV, SOC, (+), and (-) correspond to the open circuit voltage, state of charge, positive active material, and negative active material, respectively. Green, red, and blue boxes/text reflect calculations/inputs involving the positive electrode, the negative electrode, or both, respectively.

Results from the inner loop are used to complete the calculation on the outer loop. For instance, the formation losses calculated in the inner loop are used to determine the course of action in the outer loop for determining the degree of lithiation in the materials at 0% SOC (see Figure 7). The course of action depends on whether the total positive site losses (mAh) are greater than the lithium

inventory losses. Next, the degree of lithiation (x , where $x = 1$ corresponds to all sites filled) in both materials is calculated as a function of SOC. After that, the voltage of each electrode versus Li/Li^+ is determined by interpolating values from the database of x versus open circuit voltage (OCV) provided by BatPaC. The full cell voltage at 100% SOC is then compared to the target voltage and the positive, first-charge, cutoff voltage is updated.

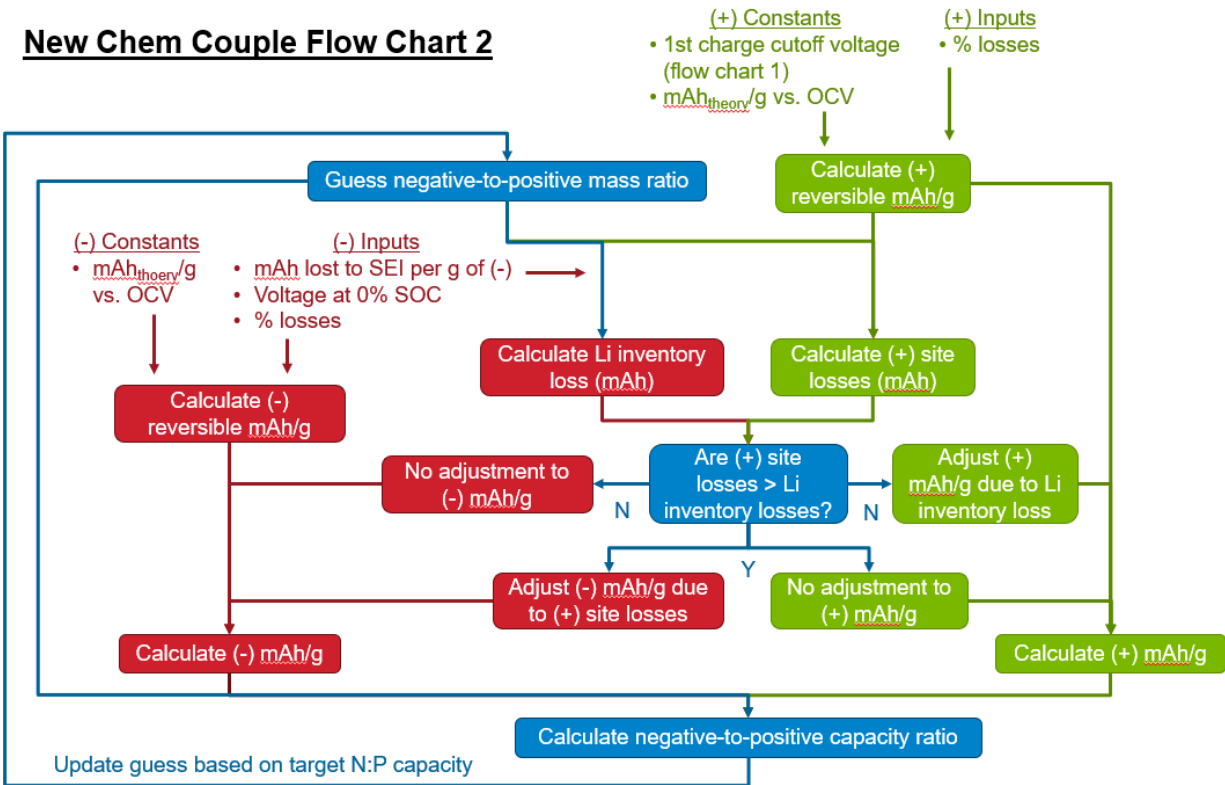


Figure 8. Flow chart describing the inner iterative loop in the calculation. The negative-to-positive (N:P) mass ratio is updated iteratively in the calculation until the N:P capacity ratio converges to the target value. OCV, SOC, (+), and (-) correspond to the open circuit voltage, state of charge, positive active material, and negative active material, respectively. Green, red, and blue boxes reflect calculations involving the positive electrode, the negative electrode, or both, respectively.